On the Stabilization of Polar Metal Oxide Surfaces:
A First Principles Study of Fe_3O_4(001)

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Magnetite is not only of substantial geological importance but also a potential material for the development of spintronic devices. However, the structure of the reconstructed (001)-surface has not been unambiguously resolved to date and is subject of a controversial debate in the literature. Using *ab initio* atomistic thermodynamics [1] we construct a phase diagram of Fe3O4(001) for a variety of stoichiometric and non-stoichiometric terminations. A modified bulk termination which has been hitherto ignored based on formal electrostatic criteria is identified as the lowest energy configuration over a broad range of oxygen pressures. The DFT-predicted geometry with octahedral iron and oxygen forming a *wave-like* structure along the [110]-direction is supported by an x-ray diffraction analysis[2]. The stabilization of the Fe3O4(001)-surface goes together with significant changes in the electronic and magnetic properties, e.g. a *halfmetal-to-metal* transition.

[1] K. Reuter and M. Scheffler, Phys. Rev. B 65, 035406, (2002) and references therein.

[2] R. Pentcheva, F. Wendler, N. Jedrecy, H.L. Meyerheim, W. Moritz, and M. Scheffler in preparation.